Solutions to Problems

CHAPTER 1

1.1. (a) Simple cubic: 1 atom per unit cell; 
\[
\frac{4}{3} \pi \frac{a^3/2}{a^3} = \frac{\pi}{6}.
\]

(b) BCC: 2 atoms per unit cell; 
\[
2 \times \frac{4}{3} \pi \frac{\sqrt{3}a^3/4}{a^3} = \frac{\sqrt{3} \pi}{8}.
\]

(c) FCC: 4 atoms per unit cell; 
\[
4 \times \frac{4}{3} \pi \frac{\sqrt{2}a^3/4}{a^3} = \frac{\sqrt{2} \pi}{6}.
\]

(d) HCP: 6 atoms per unit cell; 
\[
6 \times \frac{4}{3} \pi \frac{a^3/2}{a^3} = \frac{\sqrt{2} \pi}{6}.
\]

(e) Diamond: 8 atoms per unit cell; 
\[
8 \times \frac{4}{3} \pi \frac{\sqrt{3}a^3/8}{a^3} = \frac{\sqrt{3} \pi}{16}.
\]

1.2. (a) Base-centered tetragonal lattice is composed of the simple tetragonal lattice in which the edge length of base is equal to \(\sqrt{2}a/2\).

(b) Face-centered tetragonal is composed of the body-centered tetragonal in which the edge of base is equal to \(\sqrt{2}a/2\).

(c) Face-centered rhombohedral actually contains a simple rhombohedral in which the edge ratio of the unit cell is equal to 0.5.

1.3. A fivefold axis of symmetry cannot exist in a lattice because it is impossible to fill all the space with a connected array of pentagons.

1.4. (a) BCC: 
\[
A = \frac{a}{2} (\hat{x} + \hat{y} + \hat{z}), \quad B = \frac{a}{2} (-\hat{x} + \hat{y} - \hat{z}), \quad C = \frac{a}{2} (\hat{x} - \hat{y} - \hat{z}).
\]

(b) FCC: 
\[
A = \frac{a}{2} (\hat{x} + \hat{y}), \quad B = \frac{a}{2} (\hat{y} + \hat{z}), \quad C = \frac{a}{2} (\hat{x} + \hat{z}).
\]

1.5. (a) A unit cell of the diamond lattice is constructed by placing atoms \(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\) from each atom in a fcc.

(b) Total number of atoms per unit cell = 8; the distance is 1.54 Å; and 2.43 Å and 2.35 Å for Ge and Si, respectively.

1.6. The fcc edge is \(\sqrt{2}\times\) length of the edge and the body centers of the body-centered tetragonal become the face centers of the fcc.

1.7. (a) 4.

(b) The basis of the diamond structure consists of two atoms at (000, \(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\)). Therefore, the primitive vectors of the diamond structure are the same as those of the fcc.
1.8. The translational vectors are:

\[ \delta_1 = \left( \frac{a}{2} \right)(\hat{x} + \hat{y} - \hat{z}), \quad \delta_2 = \left( \frac{a}{2} \right)(-\hat{x} + \hat{y} - \hat{z}), \quad \delta_3 = \left( \frac{a}{2} \right)(\hat{x} - \hat{y} + \hat{z}). \]

The primitive translation vectors \( \delta_1^*, \delta_2^*, \) and \( \delta_3^* \) of the reciprocal lattice are defined by Eq. (1.5) as follows:

\[ \delta_1^* = \left( \frac{2\pi}{a} \right)(\hat{x} + \hat{y}), \quad \delta_2^* = \left( \frac{2\pi}{a} \right)(\hat{y} + \hat{z}), \quad \delta_3^* = \left( \frac{2\pi}{a} \right)(\hat{x} + \hat{z}). \]

Thus, the reciprocal lattice of a bcc is a fcc lattice.

1.9.

1.10. According to Fig. 1.7, it is found that the reciprocal lattice vectors are

\[ K = \frac{2\pi}{a} [(h - k + l)\hat{x} + (h + k - l)\hat{y} + (-h + k - l)\hat{z}] \]

where \( h, k, l \) are integers. The shortest \( K \) vectors are the eight vectors \((2\pi/a)(\pm \hat{x}, \pm \hat{y}, \pm \hat{z})\). The boundaries of a primitive cell in the reciprocal lattice are determined for the most part by these eight planes normal to these vectors at their midpoint. However, the corners of the octahedron thus formed are cut by the planes that are perpendicular bisectors of six other reciprocal lattice vectors:

\[ \frac{2\pi}{a}(\pm 2\hat{x}), \quad \frac{2\pi}{a}(\pm 2\hat{y}), \quad \frac{2\pi}{a}(\pm 2\hat{z}). \]

Therefore, the first Brillouin zone, which is the smallest volume, is enclosed by eight \{111\} and six \{200\} planes.

1.11. (a) \{100\}, \{200\} : both have six planes.
\( \{110\}, \{220\} \) : both have twelve planes.
\( \{111\} \) : eight planes.

(b) The normal distances are:
\( (100) \ a; \ (110) : \sqrt{2}a/2; \ (111) : \sqrt{3}a/3; \ (200) : 0.5a; \ (220) : \sqrt{2}a/4. \)

1.12. According to Fig. 1.4(C), \( AB = \sqrt{3}a/2; \ C = 2 \times (a^2 - (a/\sqrt{3})^2)^{1/2} = \sqrt{a}. \)
1.14. (a) Frenkel defect:

\[ P = \frac{N!}{n!(N-n)!} \cdot \frac{N'}{n!(N'-n)!} \]

And by applying Eqs. (1.14)-(1.16) and Sterling's approximation we then get the first derivative of the free energy \( F \) as follows:

\[ \frac{dF}{dn} = E_f - k_BT \ln \left( \frac{(N-n)(N'-n)}{n^2} \right) = 0 \]

where \( E_f \) is the activation energy for creating a Frenkel defect. Therefore,

\[ n = \sqrt{NN'} \exp \left( \frac{-E_f}{2k_BT} \right) \quad \text{for} \quad N \gg n, \quad N' \gg n \]

(b) Schottky defect: The proof for Schottky defect is similar to (a) except that \( P = N! / n!(N-n)! \), while \( E_c \) is the activation energy for creating a vacancy and \( E_v \) for creating a pair of vacancies for the ionic crystal. Therefore,

\[ n = N \exp \left( \frac{-E_c}{k_BT} \right) \quad \text{if} \quad N \gg n \quad \text{and} \quad n = N \exp \left( \frac{-E_v}{2k_BT} \right) \quad \text{if} \quad N \gg n \]